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Elastic collisions of intermediate energy electrons with water molecule

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Abstract: Differential, total and momentum transfer cross sections are calculated for elastic scattering of electrons by H_2O molecule using Independent-Atom-Model (IAM) over a wide energy range (100 - 1000 eV). Upto 500 eV scattering amplitudes $f(\theta)$ for H atom have been obtained in Khare-Shobha approximation (KSA) while for oxygen atom in partial waves. For incident energies $E \geq 500$ eV KSA has been used for both the atoms to calculate scattering amplitude. The present results are compared with the available experimental data and other theoretical calculations. Our results although obtained through a relatively simple approach are in good agreement with data throughout the whole angular and energy range except at 100 eV and are comparable to other theoretical calculations carried out so far.

Keywords: Independent atom model, Khare-Shobha approximation, intermediate-energy electrons, water molecule, elastic scattering, cross sections.

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1. Introduction

Elastic cross sections for $\bar{e}$-H_2O scattering process are used as a standard for determination of the inelastic cross sections and find their applications in radiation chemistry and space exploration (Danjo and Nishimura 1985). Trajmar *et al* (1983) and Gianturco and Jain (1986), respectively, have reviewed the experimental and theoretical work on electron-molecule scattering. It is evident from these survey that only a few investigations are available on $\bar{e}$-H_2O elastic collisions at intermediate energies. Lassettre and White (1973) have measured elastic DCS at 500 eV. Danjo and Nishimura (1985) have reported the same over an energy range 4 to 200 eV. Recently Katase *et al* (1986) have measured elastic DCS over a wide angular ($5° - 130°$) and energy range ($100 - 1000$ eV) for $\bar{e}$-H_2O elastic scattering. Theoretically, only the investigations of Fujita *et al* (1983) in Glauber approximation and Jain *et al* (1988) on $\bar{e}$-H_2O elastic scattering are available. In this recent investigation of Jain *et al* (1988) optical potential approach has been used

to obtain elastic DCS by taking different versions of exchange and polarisation potentials. Katase *et al* (1986) also carried out model calculation in static field. However, all these theoretical results under-estimate the data particularly at large scattering angles by a large amount.

Recently, Khare and Raj (1979, 1982) investigated $\bar{e}$-CO, $\bar{e}$-O_2 and $\bar{e}$-CO_2 elastic scattering in IAM using partial wave method in the intermediate energy region in which both direct and polarisation potential for each constituent atoms were considered. Scattering amplitudes from different atom were added coherently. This approach has yielded very encouraging results for these molecules at intermediate energies ($E > 100$ eV). Hence it may be worth while to extend the same approach to $\bar{e}$-H_2O scattering. In the present paper we report elastic differential, total and momentum transfer cross sections over the energy range (100 – 1000 eV).

2. Theory

The differential cross section (DCS) averaged over all orientations of molecular axis in independent atom model (IAM) is given by (Massey *et al* 1969)

$$I_{\text{Mol}}(\theta) = \sum_{i=1}^{N} \sum_{j=1}^{N} f_i(\theta) f_j^*(\theta) \frac{\sin Kr_{ij}}{Kr_{ij}} \tag{1}$$

where N is the number of atoms in the molecule. $f_i(\theta)$ and $f_j(\theta)$ are the scattering amplitudes proper to the i^{th} and j^{th} atom, respectively. K is the magnitude of momentum transfer by incident electron during collision. r_{ij} is the equilibrium internuclear distance between i^{th} and j^{th} atom. This equation neglects the possibility of multiple scattering and assumes that each atom scatters as if it was free.

The atomic scattering amplitude $f(\theta)$ in partial waves, taking all the partial waves into account is given by

$$f(\theta) = \frac{1}{k} \sum_{l=0}^{M} (2l+1) e^{i\eta_l} \sin \eta_l P_l (\cos \theta) + f_{dp}^{B}(\theta)$$

$$- \frac{1}{k} \sum_{l=0}^{M} (2l+1) \eta_l^B P_l (\cos \theta) \tag{2}$$

where η_l^B and $f_{dp}^{B}(\theta)$ are the phase shifts and scattering amplitude, respectively, in first Born due to the dynamic polarisation potential. P_l (cos θ) are Legendre polynomials and M is an integer.

To obtain phase shifts η_l for l^{th} partial wave the following differential equation is numerically solved (we express length in the units of a_0 and energy in Rydberg unless stated otherwise).

$$\left[\frac{d^2}{dr^2}+k^2-V_{opt}(r)-\frac{l(l+1)}{r^2}\right]f_l(r)=0 \tag{3}$$

where k^2 is the energy of the incident electron. The optical potential $V_{opt}(r)$ in general is complex energy dependent, non-local and is supposed to represent all the electron-atom interactions i.e. direct, polarization, exchange and absorption. For 10 electron targets the exchange effects have been found negligible for incident energies $E > 100$ eV (Jhanwar *et al* 1978, Jain *et al* 1988). The absorption effects are also supposed to have a little impact on the results in the energy range considered here. Therefore, in the present investigation we take $V_{opt}(r)$ as the sum of direct $V_{00}(r)$ and polarisation potential $V_{dp}(r)$ and is spherically symmetric, real, local and energy dependent. The analytical expressions of Strand and Bonham (1964) are used for static potential of the atoms. $V_{dp}(r)$ is represented by spherically symmetric and energy dependent potential given by (Jhanwar and Khare 1976)

$$V_{dp}(r)=-\frac{\alpha_d r^2}{(r^2+d^2)^3}-\frac{\alpha_q r^4}{(r^2+d^2)^5} \text{ with } d=0.75\ k/\Delta. \tag{4}$$

α_d, α_q are, respectively, dipole and quadrupole polarizabilities of the atom. Δ is the mean excitation energy of the atom and is equal to $\exp[L(-1)/S(-1)]$. $L(-1)$ and $S(-1)$ are the properties of the atom related to oscillator strength distribution taken from Dehmer *et al* (1975). For H atom α_d, α_q are taken 4.5, 15 and for O atom 5.2, 16.3, respectively. Δ is calculated as 0.925 and 2.01, respectively for H and O atoms.

It may be noted that $V_{dp}(r)$ although semi-empirical is free from any adjustable parameter. It may further be noted that the polarisation potential used by Jain *et al* (1988) [eq. 2 of this reference] does not give correct behaviour near the origin for $n=2$.

In eq. 2 we also require η_l^B. However, calculation of η_l^B for higher values of l becomes time consuming as it involves modified Bessel function. So, we have replaced it by semi-classical phase shift η_l^s, given by (LaBahn and Callaway 1969)

$$\eta_l^s=-\frac{1}{2k}\int_{r_0}^{\infty}\frac{rV_{dp}(r)dr}{[r^2-r_0^2]^{1/2}} \text{ with } r_0=l+0.5/k. \tag{5}$$

We have compared η_l^s with η_l^B for different targets and at various energies and it was found that they are within 3% (Raj 1981) and need negligible time for their

evaluation. Value of M is so chosen that at $l=M$, η_l and η_l^B are within 2%. For higher energies where this condition is not fulfilled, maximum value of M is taken to be equal to 20.

In a scattering process, there can be a situation where the distortion of the wave function of the projectile may not be of importance but the distortion of the target may be quite significant. Under such conditions the wave function of the projectile in both the channels i.e. initial and final may be taken to be a plane wave. This was proposed by Khare and Shobha (1970). So, it is also called the Khare-Shobha approximation (KSA). Main feature of this approximation is that it is computationally as simple as first Born. Scattering amplitude in KSA is given by

$$f^{\mathrm{KSA}}(\theta)=f_{B1}(\theta)+f_{ap}^{B}(\theta). \tag{6}$$

In the studies of Jain (1978), it has been found that for $E \geqslant 200$ eV KSA is successful to explain data for e-H scattering. So, the scattering amplitude $f(\theta)$ for H atom has been calculated in KSA. For oxygen atom upto 500 eV partial wave method has been employed where KSA is not expected to be successful. However, above 500 eV for oxygen atom also we use KSA. Finally $I_{\mathrm{mol}}(\theta)$ is obtained from eq. (1). The total cross section (TCS), $Q(E)$, and momentum transfer cross sections (MTCS), $Q_M(E)$, are then obtained from the following relations, respectively,

$$Q(E)=2\pi \int_0^{\pi} I_{\mathrm{mol}}(\theta) \sin\theta \, d\theta \tag{7}$$

$$Q_M(E)=2\pi \int_0^{\pi} I_{\mathrm{mol}}(\theta)(1-\cos\theta) \sin\theta \, d\theta \tag{8}$$

3. Results and discussion

Our present results of DCS are shown in Figures 1 to 3 over the energy range (100 – 1000 eV). The results of sophisticated calculation of Jain et *al* (1988) are included in figures for comparison. The Glauber results of Fujita et *al* (1983) differ with data significantly at large scattering angles ($\theta > 60$) both in magnitude and shape. Calculations of Katase et *al* (1986) have been carried out only in static field approximation hence these results are not included in figures. First of all we focus our attention at Figure 1. We see that the present results at 100 and 200 eV reproduce all the minor variations in DCS and show a dip at the same angle as observed experimentally. As far as magnitude is concerned, our values at 100 eV lie much higher than the data of Danjo and Nishimura (1985) and Katase et *al* (1986) particularly, in the middle angular range. However, this difference decreases at 200 eV. The values of Jain et *al* (1988) are in better agreement with data at

100 eV throughout the whole angular range but show a poor agreement with the data at 200 eV impact energy for $\theta > 80°$. Results of Glauber approximation (Fujita *et al* 1983) also differ from the experimental data significantly for large

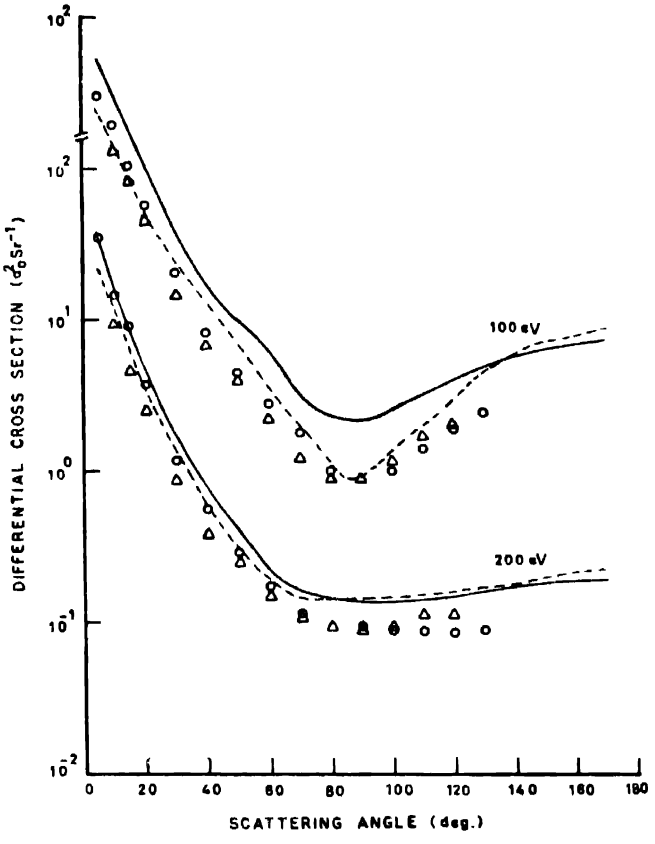

Figure 1. Elastic differential cross section for $\bar{e}$-H_2O scattering at incident energies 100 to 1000 eV (Note displacement of initial scale).
--- : Present calculations : - - - - : Jain *et al* (1988).

Experimental data :
× : Lassettre and White (1973) ; Δ : Danjo and Nishimura (1985) ;
O : Katase *et al* (1986).

scattering angles ($\theta > 60°$) both in magnitude and shape. Reason of this large difference between present results and data at 100 eV might be the neglect of the distortion of the incident electron by H atom and the multiple scattering effects within the molecule which will be significant at this energy. Inclusion of the distortion of the incident electron is expected to decrease DCS at small and middle angles but to increase it at large scattering angles whereas inclusion of multiple scattering effects will reduce DCS by a large factor at all scattering angles (Hayashi and Kuchitsu 1976, 1977, Daimon *et al* 1979).

It is evident from Figures 2 and 3 that above 200 eV, the agreement between the present values and data increases regularly and fairly good agreement is obtained at 500 eV through ut the whole angular range. At this energy our values

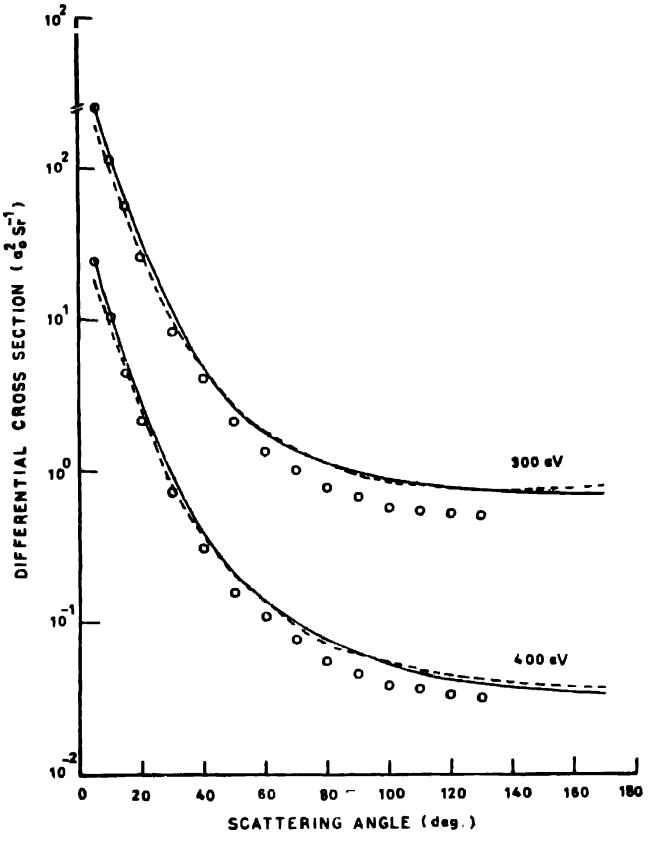

Figure 2. Elastic differential cross sections for e-H_2O scattering at incident energies 100 to 1000 eV (Note displacement of initial scale).
– : Present calculations ; - - - - : Jain *et al* (1988).
Experimental data :
× : Lassettre and White (1973) ; Δ : Danjo and Nishimura (1985) ;
O : Katase *et al* (1986).

show a good agreement with both the data of Lassettre and White (1973) and Katase *et al* (1986). It may be noted that Jain *et al* (1988) have not plotted the data of Lassettre and White (1973) correctly at 500 eV (See Figure 5 of this reference). In this figure there is a large difference between the data of Lassettre and White and Katase *et al* (1986) whereas in fact the two data are nearly equal. Above 500 eV, we calculated scattering amplitude for oxygen atom also in KSA and then DCS for H_2O at 700 and 1000 eV. These values slightly overestimate the data at low scattering angles and underestimate at large scattering angles. It

clearly indicates that the distortion of incident electron wave function is still significant even at 1000 eV by the constituent oxygen atom of the water molecule.

In Table 1 we have compared our values of total (Q) and momentum transfer (Q_M) cross sections for elastic $\bar{e}$-H_2O scattering with the available experimental

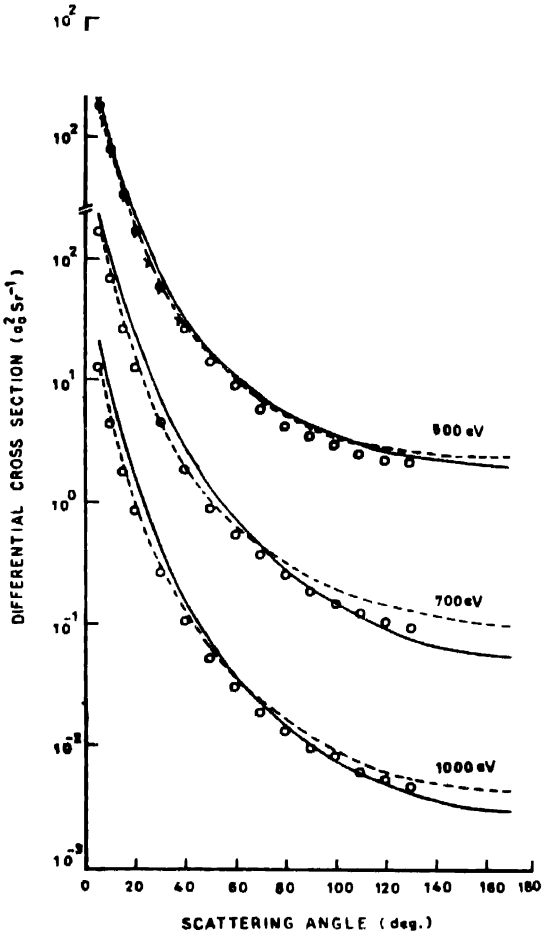

Figure 3. Elastic differential cross section for $\bar{e}$-H_2O scattering at incident energies 100 to 1000 eV (Note displacement of initial scale).
—— : Present calculations ; - - - - : Jain *et al* (1988).

Experimental data :
× : Lassettre and White (1973) ; Δ : Danjo and Nishimura (1985) ;
O : Katase *et al* (1986).

data and other theoretical calculations. It may be noted that our values of TCS obtained through a very simple approach are almost within 14% to that of Jain *et al* (1988) for impact energies $E > 200$ eV and are in good agreement with the data of Katase *et al* (1986). However, the difference for $E \leqslant 200$ eV is large due to the

already mentioned reasons. Present results for MTCS are also comparable with the results of Jain et *al* (1988) throughout the energy range investigated here and show fairly satisfactory agreement with the data of Katase et *al*. One of the reasons for small difference between the present values of Q and Q_M and data might be due to the fact that Katase et *al* have extrapolated their data beyond 130°

Table 1. Total elastic (Q) and momentum transfer (Q_M) cross sections, respectively, for electron scattering by water molecule in units of a_0^2.

Energy eV	Q				Q_M			
	Theoretical		Experimental		Theoretical		Experimental	
	Present	Jain et *al* (1988) SHP 1 Model*	*a*	*b*	Present	Jain et *al* (1988) SHP 1 Model*	*a*	*b*
100	19.76	12.03	10.64	8.46	6.39	5.57	3.61	3.08
200	9.33	7.54	7.54	5.36	2.45	2.39	1.66	1.80
300	6.48	5.68	5.57		1.39	1.36	1.06	—
400	5.11	4.64	4.71		0.92	0.90	0.74	—
500	4.29	3.96	3.71		0.66	0.65	0.56	—
700	3.27	3.07	2.92	—	0.27	0.39	0.33	—
1000	2.36	2.33	1.96		0.15	0.22	0.18	—

a– Katase et *al* (1986) ; *b*– Danjo and Nishimura (1985).

* Only the values of the most successful model (SHP 1) of Jain et *al* (1988) are included here.

and they have retained the same trend as observed at 100 and 200 eV i.e. increasing trend of DCS in backward direction. However, for $E > 200$ eV such a behaviour of DCS has not been found in theoretical calculation.

Finally, it is concluded that a relatively simple approach (Khare-Shobha approximation along with independent atom model) gives values of DCS, TCS and MTCS for e-H_2O elastic scattering comparable to those obtained by Jain et *al* (1988) through a more sophisticated approach. Inclusion of distortion of incident electron wave function by H atom at and below 200 eV and by oxygen atom for $E > 500$ eV is expected to yield better results throughout the whole energy range (100–1000 eV). The work in this direction is in progress.

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